


Numerical Analysis
Odd Semester 2024/2025
GP 1: System of Linear Equation & Least
Square Problem




Group K3:


Adam Muhammad - 2206046613
Ardhika Satria Narendra - 2206821866
Ferdinand Raja Kenedy - 2206046683
Rakha Fahim Shahab - 2206821166

“We hereby declare that this assignment is the result of our group’s own work”

Adam Muhammad - 2206046613 

Ardhika Satria Narendra - 2206821866 

Ferdinand Raja Kenedy - 2206046683 

Rakha Fahim Shahab - 2206821166 

Wolfriend's Claw Mark

Introduction	5
A. LU Factorization Methods	6
LU Factorization with Pivoting	6
Recursive LU Decomposition	7
Block LU Factorization	8
Experiment Result	8
B. Analysis of Condition Number and Error Propagation	9
Influence of Matrix Size (N)	9
Influence of Bandwidth (p and q)	9
C. Banded Matrix Experiment Result	10
D. Improvement	11
Cholesky LU Factorization	11
Computational Complexity	11
Optimized Recursive LU Factorization	12
Optimized for Tridiagonal Matrix	13
Conclusions	15
References	15

Introduction

In this task, we delve into the intricacies of numerical analysis, focusing primarily on different LU factorization methods and their efficiency in solving systems of linear equations. LU factorization serves as a cornerstone of numerical linear algebra, where matrix decomposition is utilized to facilitate the solution of linear systems, particularly in computational environments. The goal is to explore the LU Factorization with Pivoting, Recursive LU Decomposition, and Block LU Factorization to determine their computational complexities, numerical stability, and effectiveness in handling various types of matrices. Additionally, we examine how the condition number of a matrix impacts the propagation of errors, analyzing the influence of matrix size and bandwidth on numerical stability. This analysis is instrumental in understanding the suitability of each factorization technique for different matrix conditions and in optimizing the accuracy and efficiency of solving linear systems.

A. LU Factorization Methods

LU Factorization with Pivoting

LU factorization with pivoting is a modified version of the basic LU decomposition that uses row swapping to improve stability. Pivoting is used to eliminate the issues caused by small pivot elements that can make errors during the process. During the decomposition process, the algorithm finds the largest absolute pivot element from the matrix's current column, swapping the row containing this pivot with the current row. This pivot strategy can be mathematically written as $PA = LU$, where P represents the permutation matrix that records the row swaps. The use of pivoting makes the decomposition process remain well-conditioned against numerical inaccuracies.

Given Matrix A :

$$A = \begin{bmatrix} 1 & 4 \\ 3 & 2 \end{bmatrix}$$

To decompose matrix A , into matrix L and U , first observe the first column to determine the pivot. Compare the absolute value of the first column, because The element 3 in the second row is larger than 1 in the first row, so swap the first and second rows. After the swapping process, then matrix A become:

$$A = \begin{bmatrix} 3 & 2 \\ 1 & 4 \end{bmatrix}$$

Next, update the second row by:

$$R2 = R2 - \frac{1}{3} \times R1$$

After transforming the first column of the second row into 0, then matrix A become:

$$A = \begin{bmatrix} 3 & 2 \\ 0 & \frac{10}{3} \end{bmatrix}$$

Because A is already an upper triangular matrix, therefore matrix we have matrix U :

$$U = \begin{bmatrix} 3 & 2 \\ 0 & \frac{10}{3} \end{bmatrix}$$

Then, matrix L is composed of the multipliers used in the elimination process. Therefore, we have matrix L :

$$L = \begin{bmatrix} 1 & 0 \\ \frac{1}{3} & 1 \end{bmatrix}$$

Lastly, for permutation matrix P , it reflects the initial row swap, which leads to matrix P :

$$P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Recursive LU Decomposition

Recursive LU decomposition is a concept which breaks down the decomposition problem into smaller and simpler parts. It is generally very effective at large matrix problems, using the divide-and-conquer strategy to enhance performance of the decomposition process. The process is to split the matrix into smaller and smaller sub-matrices until it reaches the base case, where the sub-matrix is small enough-for instance, 1×1 -and can be solved directly.

To apply this method, consider a matrix A of size $n \times n$. Next, the matrix is recursively decomposed into four submatrices $A_{11}, A_{12}, A_{21}, A_{22}$. Next, for each matrix, it will be recursively decomposed into another four submatrices until it reaches the base case, or 1×1 matrix.

For the detailed steps, given matrix A , matrix A is divided into four blocks. The top-left block A_{11} and the bottom-right block A_{22} are square matrices of size $\lfloor \frac{n}{2} \rfloor \times \lfloor \frac{n}{2} \rfloor$. A_{12} and A_{21} are the remaining blocks that complete the matrix A .

Then, apply recursive LU decomposition to A_{11} , which will result into L_{11} and U_{11} . Next, solve L_{12} and U_{21} by using the relations $L_{12} = L_{11}^{-1} \times A_{12}$ and $U_{21} = A_{21} \times U_{11}^{-1}$. Then, compute the Schur complement of A_{22} relative to A_{11} , which is $A_{22} - U_{21} \times L_{12}$. This Schur complement will focus on the remaining part of the matrix that needs to be factorized. Finally, The matrix L is assembled from L_{11}, L_{12}, U_{21} , and L_{22} and the matrix U is formed from U_{11}, L_{12}, U_{21} and U_{22} .

Block LU Factorization

Block LU factorization is a matrix decomposition technique that partitions a matrix into smaller block matrices, which are then factored using the LU decomposition method. This approach is effective for large matrices where computational efficiency is something to keep in mind.

In block LU factorization, the matrix A is divided into smaller square blocks, and the LU decomposition is applied to these blocks rather than the entire matrix. This decomposition results in matrices L and U , where L is lower triangular with block structure, and U is upper triangular. The factorization process involves iterative updates to these blocks, systematically transforming the original matrix into a format where the blocks of L and U directly correspond to the blocks of A .

The effectiveness of block LU factorization depends heavily on the size and number of blocks, which should be chosen based on the properties of the matrix to ensure optimal performance.

Experiment Result

```
octave:17> test2()

Testing LU methods for 11 x 11 matrix:
LU Pivoting: Time = 0.0021 s, FLOPs = 887
Recursive LU: Time = 0.0021 s, FLOPs = 356
Block LU: Time = 0.0002 s, FLOPs = 887

Testing LU methods for 8 x 8 matrix:
LU Pivoting: Time = 0.0011 s, FLOPs = 341
Recursive LU: Time = 0.0013 s, FLOPs = 168
Block LU: Time = 0.0001 s, FLOPs = 341

Testing LU methods for 10 x 10 matrix:
LU Pivoting: Time = 0.0015 s, FLOPs = 667
Recursive LU: Time = 0.0013 s, FLOPs = 306
Block LU: Time = 0.0001 s, FLOPs = 667

Testing LU methods for 18 x 18 matrix:
LU Pivoting: Time = 0.0044 s, FLOPs = 3888
Recursive LU: Time = 0.0021 s, FLOPs = 1858
Block LU: Time = 0.0001 s, FLOPs = 3888

Testing LU methods for 9 x 9 matrix:
LU Pivoting: Time = 0.0010 s, FLOPs = 486
Recursive LU: Time = 0.0010 s, FLOPs = 200
Block LU: Time = 0.0001 s, FLOPs = 486
octave:18>
```

Figure A.1

Result of the experiment

As can be seen from the result of the experiment, we can see that Block LU decomposition proves to be the fastest method in 5 random matrix sizes. It also can be inferred that recursive LU decomposition has the least FLOPS count than other methods. This shows how recursive LU decomposition enhances the performance of the decomposition into smaller problems. As for the LU factorization with pivoting shows a moderate result based on the experiment.

B. Analysis of Condition Number and Error Propagation

The condition number of a matrix helps determine how sensitive the matrix is to numerical errors, which eventually influences the stability of the solution from the use of LU factorization. This is done in order to study how well or ill-conditioned the matrix is by computing the condition number for every combination of matrix size N , lower bandwidth p , and upper bandwidth q . The larger the condition number, the more sensitive the matrix is to the propagation of errors; that is, the larger the relative perturbation in the solution caused by a given relative perturbation in the input data.

Matrices with condition numbers that are within the range $1 \leq \text{cond}(A) \leq 10^3$ are well-conditioned, where the numerical errors are minimal and where a correct solution can be determined accurately. In cases where the condition numbers happen to fall between 10^4 and 10^6 , the matrix is moderately ill-conditioned; that is, though errors might arise, the system remains solvable but not with too much accuracy. If the condition number is larger than 10^6 , then this means that a matrix is highly ill-conditioned; huge error propagation occurs, and the solution can be far from the truth. Then, more numerically stable techniques such as LU factorization with pivoting become necessary to suppress the effects of the ill-conditioning.

Influence of Matrix Size (N)

As the matrix size N increases, the condition number tends to rise, particularly when the matrix has a large bandwidth. This relationship highlights that larger matrices are more prone to being ill-conditioned, especially when coupled with wider bandwidths (p and q). In these cases, the system becomes more sensitive to numerical errors, and solving such systems accurately requires stable algorithms. LU factorization with pivoting, for instance, helps address these stability concerns by reordering rows to ensure large pivot elements, thereby reducing numerical errors during the factorization process.

Influence of Bandwidth (p and q)

The bandwidth parameters p and q directly influence the matrix's condition number. Larger values of p and q introduce more non-zero elements around the diagonal of the matrix, which increases the condition number and, consequently, the likelihood of error propagation. A matrix with a wide bandwidth may become ill-conditioned, leading to less accurate solutions. Conversely, narrow bandwidths (smaller p and q) typically result in better-conditioned matrices. In such cases, fewer non-zero elements around the diagonal contribute to greater numerical stability and minimize the chances of error propagation, making the solution more reliable.

C. Banded Matrix Experiment Result

In this part, we compare the performance of three LU decomposition methods—Standard LU Pivoting, Recursive LU, and Block LU—by evaluating computational complexity, represented by Floating Point Operations (FLOPs), and accuracy, indicated by residual norms. Our analysis focused upon the findings before, which highlighted the influence of matrix size and bandwidth on the condition numbers and the effect of errors in matrix.

About the influence of the size of the matrix, it can be seen that when the size increases, the condition numbers are higher and this means more numerical instability. This phenomenon was the same for all the decomposition methods tested, where the outcomes developed for larger matrices tended to result in higher residuals and thus gave a mirror image of the numerical errors. Other parameters influential in defining the condition number of a matrix in this context are bandwidth parameters, p and q . Larger values of these parameters will raise the condition number, which in turn raises the chance that an error during a calculation will be propagated. This was a common finding with matrices of wider bandwidths, where less numerical stability was measured.

Compared to performance metrics, Standard LU Pivoting typically shows moderate computational times for the varying sizes of matrices involved while also having higher residuals than Recursive LU did, particularly for larger-sized matrices with increased bandwidth..

Recursive LU often gives the smallest residuals of the methods compared and thus appears to have the best numerical accuracy. The performance in FLOPs for this method was similar to Standard LU, since both have theoretically similar computational complexities, on the order of $\frac{2}{3}N^3$ FLOPs.

Block LU commonly gives the least execution times. On the other hand, this method usually gives the highest residuals, especially for those cases with big bandwidths and size of matrices involved.

On the other hand, it clearly follows that in most conditions of matrix size and bandwidth, Recursive LU has given essentially the best trade-off between computational efficiency and accuracy. Which of these decomposition methods to apply would again be based on what a certain application requires: Standard LU Pivoting, when numerical stability in ill-conditioned matrices is required; Recursive LU, for applications where time efficiency with high precision is required; Block LU, for those requiring high speed with a slight compromise in accuracy.

D. Improvement

Cholesky LU Factorization

The matrix A is assumed to be symmetric and positive definite, and the parameter p represents the bandwidth, which also means the width of elements that are not zero. The function initializes a matrix L of the same dimensions as A with all elements set to zero. Then, the next process will be using a nested loop.

For the outer loop, it iterates over each i row from matrix A , from 1 until n , where n is the total number of rows or columns of matrix A . In the inner loop, for each row i , the inner loop iterates over the columns j , starting from the maximum value between 1 and $i - p$, until i . This ensures that the computations are restricted within the specified bandwidth p .

When i equals j , the diagonal element $L(i, i)$ is computed. This involves summing the squares of the elements in the i^{th} row of L , from the start of the row or from $i - p$ to $i - 1$. The diagonal element $L(i, i)$ is then determined by taking the square root of $A(i, i)$ minus this sum. For $i \neq j$, the off-diagonal elements $L(i, j)$ are computed. This process subtracts the product sum of elements in the i^{th} and j^{th} rows of L , up to the $j - 1^{th}$ element, from $A(i, j)$. The result is then divided by the diagonal element $L(j, j)$, to make matrix L remains lower triangular.

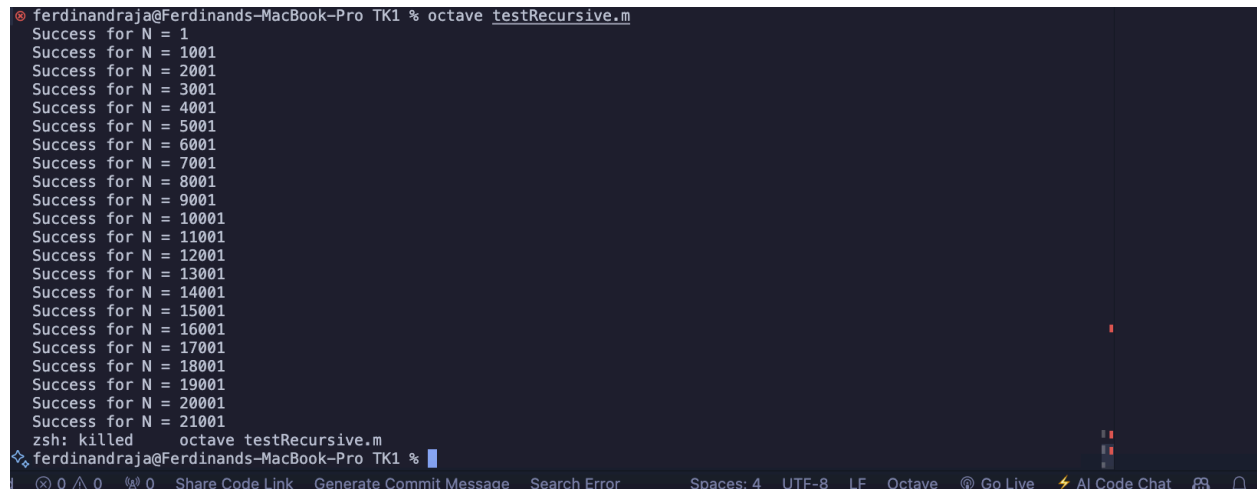
Computational Complexity

The computational complexity of the cholesky function is affected by the value of bandwidth p . Each diagonal calculation involves approximately $2p$ (flops), derived from p multiplications and $p - 1$ additions, along with the square root operation. In contrast, each off-diagonal calculation within the bandwidth necessitates about $2p + 1$ flops, considering p multiplications and additions, and one division.

Considering each row has $p + 1$ elements to compute (including both diagonal and off-diagonal), the total operations per row approximate to $2p + p(2p + 1) = 2p^2 + 3p$. Therefore, for all n rows, the overall complexity is $O(n(2p^2 + 3p))$. Given that p is significantly smaller than n for banded matrices, this complexity is substantially lower than the $O(n^3)$ required for a dense matrix decomposition, showcasing the efficiency of the function for matrices with limited bandwidth.

This specialized approach underscores the importance of algorithmic adaptation to matrix structure in enhancing computational efficiency and reducing operational overhead in numerical computations.

Optimized Recursive LU Factorization

A terminal window on a MacBook Pro showing the execution of an Octave script named 'testRecursive.m'. The script tests recursive LU factorization for matrix sizes N from 1 to 21001 in increments of 100. The output shows 'Success for N = ' followed by the value for each iteration. The process successfully completes for N=21001. However, the next line shows 'zsh: killed octave testRecursive.m', indicating a crash. The terminal window has a dark background and a light-colored text. The bottom status bar shows 'Spaces: 4 UTF-8 LF Octave @ Go Live AI Code Chat'.

Picture D.1

Normal Recursive code crash at $N > 21000$

By using the normal recursive method, it can be seen that the process returns error when the size of the matrix exceeds 21000. Because each recursive call to RecursiveLU involves creating multiple submatrices (A_{11} , A_{12} , A_{21} , A_{22}) and intermediate matrices (L_{12} , U_{21}). This process is memory-intensive, as it involves storing several copies of various portions of the matrix A at each level of recursion. For large matrices, this can lead to excessive memory consumption, potentially exhausting available system or application-specific memory resources. Therefore, to optimize the recursive LU factorization, the new recursive approach will introduce a combination approach for the process, with the direct application of standard LU decomposition.

```

1 function testRecursive()
2     maxN = 100000000000; % Adjust as needed to find the crash point
3     for N = 1:1000:maxN
4         try
5             A = rand(N, N); % Generate a random N x N matrix
6             [L, U] = recursiveLU2(A);
7             disp(['Success for N = ', num2str(N)]);
8         catch ME
9             disp(['Failed at N = ', num2str(N)]);
10            disp(getReport(ME));
11            break;
12        end
13    end
14 end

```

```

Success for N = 11001
Success for N = 12001
Success for N = 13001
Success for N = 14001
Success for N = 15001
Success for N = 16001
Success for N = 17001
Success for N = 18001
Success for N = 19001
Success for N = 20001
Success for N = 21001
Success for N = 22001
Success for N = 23001
Success for N = 24001
zsh: killed  octave testRecursive.m
zsh: ferdinandrja@Ferdinands-MacBook-Pro TK1 %

```

Picture D.2

Hybrid Recursive crash at $N > 24001$

By setting a threshold matrix size n , such as 256 in this case, the algorithm determines when to switch from recursive decomposition to standard LU, based on the submatrix sizes encountered during recursion. This strategy is particularly effective in balancing the recursive benefits of smaller submatrices with the straightforward nature of standard LU decomposition, optimizing performance across different stages of the factorization process.

Optimized for Tridiagonal Matrix

To make it more efficient in handling tridiagonal matrix Thomas Algorithms, we can take advantage of the structure to simplify operations and reduce computational complexity. Because the tridiagonal matrix only has its non-zero element in the 3 main diagonals, we can take advantage of it to make it more efficient. It first follows initializations of L to an identity matrix of size $n \times n$ and U as a zero matrix in which it gets replaced element-by-element during the decomposition process. For each row i , the algorithm first updates the diagonal element of U by subtracting the product of corresponding values in L and U from the original value in A . Then, it sets the upper diagonal of U as the value from A because these values remain unchanged through the process of decomposition for tridiagonal matrices. Meanwhile, the algorithm calculates the lower diagonal elements of L by dividing its corresponding value in A by the diagonal element of U . Iteratively, this proceeds through all rows. The result of this is an efficiently computed LU decomposition

without operations on unnecessary zero elements, thus keeping the computational complexity reduced from a general approach to perform the LU decomposition.

The Pseudocode:

1. Input:

- Matrix A (must be tridiagonal)
- n = size of the matrix (i.e., A is $n \times n$)

2. Output:

- Lower triangular matrix L
- Upper triangular matrix U

3. Initialize:

- L as an identity matrix of size n
- U as a zero matrix of size n

4. For each row i from 1 to n do:

- Step 1: Update U for diagonal elements:
 - Set $U[i, i] = A[i, i] - L[i, i-1] * U[i-1, i]$ (only if $i > 1$)
- Step 2: Update U for the upper diagonal elements (if $i < n$):
 - Set $U[i, i+1] = A[i, i+1]$
- Step 3: Update L for the lower diagonal elements (if $i < n$):
 - Set $L[i+1, i] = A[i+1, i] / U[i, i]$

5. End For

6. Return:

- L, U

For the FLOPS complexity, first we need to count how many FLOPS operations we need to count each $U[i, i]$. To calculate each $U[i, i]$, we need at most one multiplication and one subtraction, so the total number of operations are $2 * (n-1)$. Because the upper diagonals are directly taken from the main matrix, therefore there's no FLOPS operations involved. For the lower diagonal, we need 1 division for each, therefore there are $(n-1)$ operations. In total, there are $3(n-1)$ operations and can be simplified as $O(n)$.

Conclusions

In conclusion, this study provides a comprehensive exploration of various LU factorization methods, including LU Factorization with Pivoting, Recursive LU Decomposition, and Block LU Factorization, analyzing their efficiency, numerical stability, and suitability for different types of matrices. The results demonstrate that Block LU decomposition is the fastest approach for random matrices of varying sizes, while Recursive LU Decomposition proves to be the most effective in reducing the floating-point operations (FLOPs) count. LU Factorization with Pivoting, on the other hand, offers a more stable approach, making it suitable for ill-conditioned matrices. The analysis of condition numbers highlights the influence of matrix size and bandwidth on numerical stability, indicating that larger matrices and wider bandwidths tend to increase the condition number, thus requiring more numerically stable methods like pivoting to mitigate error propagation. To conclude, each method has its own advantages, with Block LU being optimal for computational speed, Recursive LU for accuracy, and LU with Pivoting for handling ill-conditioned cases.

References

BYJU'S. (n.d.). Cholesky Factorization. <https://byjus.com/maths/cholesky-factorization/>

Gotta Catch 'Em All!

Introduction.....	15
Impact of Storing Q in the QR Algorithm.....	16
Optimal K calculation for PCA.....	16
Eigenvalue Calculation.....	17
Constructing the Transformation Matrix V_k	18
Mathematical Interpretation:.....	18
Importance of Orthogonality:.....	19
Accuracy of Eigenvector Calculation.....	20
Analyzing the Residual Norm Output Results.....	21
1. Normal Equation.....	22
2. QR Decomposition.....	22
3. QR Decomposition with Stored Q.....	23
FLOPs Complexity for PCA and Linear Regression.....	23
FLOPs Calculation for PCA.....	23
PCA using QR Decomposition:.....	23
PCA using Eigenvalue Decomposition:.....	24
FLOPs Calculation for Linear Regression.....	24
Linear Regression using Normal Equation:.....	24
Comparison of Model Accuracy Before and After the Outliers Removed.....	25
Effect of Outliers on Regression:.....	25
Effect on Residual Error Norm:.....	26
References.....	28
Conclusion.....	30

Introduction

In this task, we explore the application of Principal Component Regression (PCR) as a method for dimensionality reduction and regression analysis, emphasizing the impact of outliers on model performance. PCR combines Principal Component Analysis (PCA) with linear regression, allowing us to reduce the number of features while retaining the most important variance in the data. We analyze the effect of outlier removal on the residual errors and accuracy of the model, re-running the regression with an outlier-free dataset. By comparing the results before and after removing outliers, we seek to understand how extreme data points can distort the principal components, regression coefficients, and residual norm. This study ultimately aims to demonstrate the importance of preprocessing steps, such as outlier detection and removal, in enhancing the robustness and reliability of regression models.

Impact of Storing Q in the QR Algorithm

The storing of the orthogonal matrix Q in the process of QR decomposition plays an important role in maintaining the computational processes of eigenvalues and eigenvectors as accurate. The matrix Q contains the sequence of orthogonal transformations, such as Householder reflectors, which were applied to the original matrix in a QR decomposition. Storage of Q is one of the most important factors in the maintenance of orthogonality and in tracking the intermediate transformations necessary for building the final eigenvectors.

With Stored Q : Storage of Q is essentially to be done in order to keep the record of the cumulative transformations applied in the QR process. Each Householder transformation is encoding a sequence of rotations or reflections, and the orthogonal matrix Q keeps track of those operations. In case of storing Q , it will be able to give out the eigenvectors from the final upper triangular matrix, once the iterative process converges. In this case, the orthogonality of the eigenvectors is preserved, which is important for the numerical stability of the method. Besides, storing Q minimizes the accumulation of rounding errors during iterative steps and hence enhances the accuracy of the computation of the eigenvectors.

Without Stored Q : In this case, recovering the eigenvectors is hard without storing Q . Since QR decomposition without Q only resolves to find the eigenvalues from the diagonal elements in the last matrix, the further process of the upper triangular form can't deduce the eigenvectors without recording the orthogonal transformations. This is because the eigenvectors depend on the actual sequence of steps taken to arrive at the final matrix. Secondly, its not keeping Q can lead to numerical instability because, with every iteration, the rounding error makes it possible that the orthogonal properties of the transformations are destroyed.

Optimal K calculation for PCA

The Principal Component Analysis (PCA) is a dimensionality reduction technique that transforms the data by projecting it onto a smaller set of principal components that capture the most variance in the data. One key aspect of PCA is determining the optimal number of components k that balances the dimensionality reduction with the retention of as much variance as possible.

Steps we took to calculate optimal K :

1. Calculate Covariance Matrix

Given the standardized data matrix X_{std} of size $n \times m$ (where n is the number of samples and m is the number of features), the covariance matrix Σ is calculated as:

$$\Sigma = \frac{1}{n-1} X_{std}^T X_{std}$$

2. Calculate Eigen values

Use eigen decomposition methods whether it is using QR decomposition with or without storing Q or not using QR decomposition to extract eigen values and vectors.

3. Calculate cumulative variance

The cumulative explained variance helps determine how much of the total variance is captured by the top k principal components.

Let $\lambda_1, \lambda_2, \dots, \lambda_m$ represent the sorted eigenvalues (from largest to smallest), and let λ_{total} be the sum of all eigenvalues:

$$\text{Cumulative Explained Variance for } k \text{ components} = \sum_{i=1}^k \lambda_i$$

$$\lambda_{\text{total}} = \sum_{i=1}^m \lambda_i$$

4. Choosing optimal K

The optimal number of principal components k is chosen by selecting the smallest k such that the cumulative explained variance exceeds a given threshold. For example, we decided on 90% of the variance, we choose the smallest k for which:

$$\frac{\sum_{i=1 \text{ to } k} \lambda_i}{\lambda_{\text{total}}} \geq 0.90$$

Eigenvalue Calculation

With Stored Q : Storage of Q has a less direct consequence on the computation of eigenvalues because eigenvalues are usually acquired from the entries of the diagonal matrix in the converged state subsequent to QR iterations. However, keeping Q in the decomposition of QR enhances robustness in iteration, especially in computations that deal with ill-conditioned matrices. The ill-conditioned matrices are highly sensitive, even to minor perturbations, which retaining Q helps to avoid huge deviations under such circumstances while computing the eigenvalues.

Without Stored Q : Even without storing Q , the QR algorithm can still produce the correct eigenvalues because they are derived from the diagonal elements of the matrix after sufficient iterations. However, the lack of Q may lead to a less stable process, especially for matrices that are poorly conditioned. Without the preservation of orthogonality, inaccuracies can emerge over multiple iterations, especially when the matrix's conditioning makes it susceptible to numerical errors.

Normal Equation Calculation: For normal linear regression we did not use any QR decomposition. Can Eigenvectors and Eigenvalues Be Found Without Storing Q ?

Eigenvalues: Well, eigenvalues can be computed without storing Q because it's derived from the diagonal elements of the matrix once the QR iteration has converged. However, not storing Q may reduce numerical stability, especially in the context of big or ill-conditioned matrices, where errors could propagate throughout an iterative process.

Eigenvectors: No, it is not possible to compute the eigenvectors with accuracy without storing Q . The eigenvectors depend on this history of orthogonal transformations applied to the matrix,

and these are encoded by Q . Without Q , there is no record of the transformations, hence impossible reconstruction of eigenvectors. Consequently, all computations of eigenvectors would be futile if Q were not stored.

Briefly, applying QR to PCA, the orthogonal matrix Q must be stored to correctly compute the eigenvectors, since it keeps the history of successive orthogonal transformations giving principal components. Although one can calculate eigenvalues directly without storing Q , one runs into numerical instability with the neglect of Q in such matrices that are not well-conditioned, since tiny errors lead to huge inaccuracies. Especially for high-dimensional data analysis, such as PCA, it is highly recommended to store Q during iteration for both stability and precision.

Constructing the Transformation Matrix V_k

Once the number of principal components k is selected, the transformation matrix V_k is constructed by taking the **first k eigenvectors** corresponding to the largest eigenvalues. These eigenvectors represent the new axes (principal components) onto which the data will be projected.

Mathematical Interpretation:

The transformation matrix V_k is a matrix whose columns are the eigenvectors associated with the largest eigenvalues:

$$V_k = [e_1, e_2, \dots, e_k]$$

Where:

- e_1, e_2, \dots, e_k are the eigenvectors corresponding to the largest eigenvalues.
- Each eigenvector represents a direction in the transformed space (i.e., a principal component).

These eigenvectors are orthogonal, ensuring that the principal components are uncorrelated, which is a key characteristic of PCA.

Importance of Orthogonality:

The orthogonality of the principal components (eigenvectors) ensures that the transformed data is linearly independent. This is critical in reducing multicollinearity, which is a common problem in regression analysis when the predictor variables are correlated. By projecting the data onto orthogonal principal components, we minimize redundant information and improve the efficiency of subsequent analysis.

Analysis of Linear Regression Approaches:

In addressing Problem 2a, point iv, we compare three distinct methods for performing linear regression on the transformed dataset obtained from Principal Component Analysis (PCA): The Normal Equation, QR Decomposition using Householder Transformation, and QR Decomposition with stored Q. Each method is evaluated based on its computational efficiency, numerical stability, and suitability for regression analysis in the context of dimensionality reduction.

Normal Equation

The Normal Equation represents a classical approach to linear regression, providing a closed-form solution by minimizing the least-squares cost function. Specifically, the regression coefficients β are computed as $(X^T X)^{-1} y$, where X is the transformed dataset in the principal component space, and y is the target vector. This approach is computationally efficient for datasets with a small number of features, as it allows for direct computation of the regression coefficients. However, the computational complexity of the matrix inversion, which is $O(n^3)$, poses significant challenges when dealing with high-dimensional datasets or large values of n .

Moreover, the numerical stability of the Normal Equation depends heavily on the conditioning of the matrix $X^T X$. In cases where the feature matrix exhibits multicollinearity, $X^T X$ becomes ill-conditioned, leading to large numerical errors in the inversion process. These errors can propagate through the computation of regression coefficients, resulting in unreliable estimates. Therefore, while the Normal Equation is straightforward to implement, its reliance on matrix inversion limits its applicability to situations where the dataset is well-conditioned and the dimensionality is relatively low.

QR Decomposition Using Householder Transformation

The QR Decomposition offers an alternative approach to linear regression that avoids the direct inversion of the matrix $X^T X$. Instead, the feature matrix X is factorized into an orthogonal matrix Q and an upper triangular matrix R using Householder transformations. The resulting system of equations, $QR\beta = y$, can be efficiently solved through back-substitution after transforming the target vector using $Q^T y$. The computational complexity of this decomposition is still $O(n^3)$, similar to the Normal Equation, but it provides a more numerically stable solution due to the orthogonal nature of the matrix Q .

Householder transformations work by generating a series of orthogonal reflectors that systematically zero out elements below the diagonal of the matrix, ultimately producing the upper triangular matrix R . This method inherently maintains the orthogonality of the feature transformations, which reduces the risk of error accumulation and improves the stability of the regression solution. By avoiding the explicit inversion of $X^T X$, QR decomposition minimizes the

numerical inaccuracies associated with poorly conditioned matrices, making it a more suitable choice for high-dimensional regression problems where preserving numerical accuracy is crucial.

QR Decomposition with Stored Q (Householder Transformation)

The approach of QR Decomposition with stored Q further enhances the accuracy and stability of the linear regression process by retaining the orthogonal matrix Q throughout the decomposition. During the iterative QR decomposition process, Q captures the cumulative orthogonal transformations applied to the feature matrix. By storing Q, we maintain a record of these transformations, which can then be utilized to accurately compute both the eigenvalues and eigenvectors of the transformed data. This is particularly important when the dataset has high dimensionality or when the principal components are used in regression analysis.

Storing Q significantly improves the numerical stability of the regression model, as it ensures that the orthogonal transformations are preserved throughout the computations. This stability is especially beneficial when dealing with large datasets or high-dimensional covariance matrices, where small rounding errors can accumulate and lead to substantial inaccuracies in both the regression coefficients and the predicted values. Furthermore, the orthogonal nature of Q helps mitigate the effects of multicollinearity by ensuring that the transformed features are linearly independent, leading to a more robust and reliable regression model.

The computational complexity of QR decomposition with stored Q remains $O(n^3)$ for the factorization process, similar to the other methods, but the additional memory required to store Q is justified by the benefits in numerical stability and accuracy. This method is particularly suitable for applications involving PCA, where the number of features has been reduced, but numerical precision is still paramount for obtaining meaningful regression results. By preserving orthogonality, the regression coefficients obtained through this approach are more reliable, especially when predicting outcomes from transformed datasets.

Accuracy of Eigenvector Calculation

The residual norm is used to evaluate the accuracy of the linear regression model after performing Principal Component Analysis (PCA). To quantify the error, we compute the norm of the residual vector, also known as the L2 norm or Euclidean norm.

$$\begin{aligned}\text{Residual Norm} &= \|y - \hat{y}\|_2 = \sqrt{\sum_{i=1}^n (y_i - \hat{y}_i)^2} \\ r &= y - \hat{y} = y - Z_{\text{aug}} \theta \\ Z_{\text{aug}} &= [1 \mid Z]\end{aligned}$$

Analyzing the Residual Norm Output Results

After running the linear regression models using three different approaches Normal Equation, QR Decomposition without stored Q, and QR Decomposition with stored Q the residual norms were computed as follows:

Residual (Normal Equation): 150.44600150.44600

Residual (QR Decomposition): 106.28570106.28570

Residual (QR with stored Q): 106.28570106.28570

Normal Equation:

The residual norm for the Normal Equation approach is 150.44600, which is significantly higher compared to the QR decomposition methods. This indicates that the Normal Equation results in a less accurate fit, potentially due to numerical instability, particularly when inverting the matrix $Z_{aug}^T Z_{aug}$, which may be ill-conditioned.

QR Decomposition (Without Stored Q):

The residual norm for both QR Decomposition with and without stored Q is 106.28570, which is lower than the Normal Equation. This method avoids matrix inversion and relies on the QR factorization, which is more numerically stable, leading to a better fit.

Analyzing the efficiency of Different Regression Methods

In this analysis, we compare the computational efficiency of three different methods used in Principal Component Regression (PCR): Normal Equation, QR Decomposition, and QR Decomposition with stored Q. The time taken by each method is as follows:

Time (Normal Equation): 0.00543 seconds

Time (QR Decomposition): 0.00345 seconds

Time (QR with stored Q): 0.00415 seconds

The analysis focuses on both computational performance and the practical implications of using each method in terms of accuracy and numerical stability.

1. Normal Equation

The Normal Equation method took 0.00543 seconds, which is the slowest among the three methods. The Normal Equation approach involves solving the equation:

$$\beta = (X^T X)^{-1} X^T y$$

This method is computationally expensive, particularly when dealing with large datasets or a high number of features. The computation of the inverse of the matrix $X^T X$ is the main reason for its relative inefficiency, as matrix inversion has a complexity of approximately $O(n^3)$. This leads to increased computational time, especially for larger matrices, making it impractical for high-dimensional data.

Furthermore, the Normal Equation can be numerically unstable if $X^T X$ is ill-conditioned, which often occurs when there is multicollinearity among the features. Ill-conditioned matrices amplify numerical errors during inversion, leading to less reliable results. This numerical instability, combined with the higher computational time, makes the Normal Equation less favorable for large or complex datasets.

2. QR Decomposition

The QR Decomposition method took 0.00345 seconds, which is the fastest among the three methods. This approach solves the least squares problem by decomposing the matrix X into an orthogonal matrix Q and an upper triangular matrix R :

$$X=QR$$

This decomposition allows us to solve the system by computing:

$$\beta=R^{-1}Q^T y$$

The QR Decomposition method avoids the direct computation of a matrix inverse, which improves both efficiency and numerical stability. By reducing the complexity of the inversion process, QR decomposition is often more efficient than the Normal Equation for large datasets. Its complexity is approximately $O(n^2)$, which explains why it is faster in this scenario.

Another important advantage is numerical stability. The QR decomposition is typically more robust to numerical errors compared to the Normal Equation because it does not involve explicitly computing the inverse of $X^T X$. The orthogonal matrix Q helps maintain numerical precision during calculations, particularly for ill-conditioned matrices, making this method more suitable for datasets with correlated features.

3. QR Decomposition with Stored Q

The QR Decomposition with stored Q took 0.00415 seconds, which is slightly slower than QR decomposition without storing Q . The main difference between this approach and the standard QR decomposition is that it retains the orthogonal matrix Q throughout the computation process.

Storing Q has several implications:

- **Computational Trade-off:** Although storing Q introduces additional computational overhead, as evidenced by the increase in time compared to standard QR decomposition, the trade-off is often worthwhile for ensuring accuracy and robustness. In scenarios where accuracy and the preservation of orthogonality are critical, the QR decomposition with stored Q is a suitable compromise between efficiency and reliability.

In summary, the QR Decomposition is the fastest method, demonstrating the benefits of avoiding matrix inversion, while the QR Decomposition with stored Q provides improved numerical stability and accuracy at a slight computational cost. The Normal Equation is the least efficient and potentially unstable, which limits its practical use in large or complex datasets. For most regression tasks, particularly those involving high-dimensional data or requiring accuracy in eigenvector calculation, the QR Decomposition with stored Q is recommended due to its balance of efficiency and reliability.

FLOPs Complexity for PCA and Linear Regression

FLOPs Calculation for PCA

PCA using QR Decomposition:

For covariance matrix calculation :

$$\text{FLOPs} = O(m^2n) = 2nm^2$$

For QR Decomposition

$$\text{FLOPs} = O(2nm^2 - \frac{2}{3}m^3)$$

Total FLOPs for PCA using QR Decomposition:

$$\text{Total FLOPs} = 2m^2n + (2nm^2 - \frac{2}{3}m^3)$$

PCA using Eigenvalue Decomposition:

For covariance matrix calculation :

$$\text{FLOPs} = O(m^2n) = 2m^2n$$

For eigenvalue decomposition

$$\text{FLOPs} = O(\frac{10}{3}m^3)$$

Total FLOPs for PCA using Eigenvalue Decomposition:

$$\text{Total FLOPs} = 2m^2n + \frac{10}{3}m^3$$

FLOPs Calculation for Linear Regression

Linear Regression using Normal Equation:

For $X_{\text{aug}}^T X_{\text{aug}}$ Computation:

$$\text{FLOPs} = O(m^2n) = 2m^2n$$

For inverse of $X_{\text{aug}}^T X_{\text{aug}}$:

$$\text{FLOPs} = O(m^3) = 2m^3$$

For Computing $X_{\text{aug}}^T y$:

$$\text{FLOPs} = O(mn) = 2mn$$

Total FLOPs

$$\text{Total FLOPs} = 2m^2n + 2m^3 + 2mn$$

Linear Regression using QR Decomposition:

For QR decomposition of X_{aug} :

$$\text{FLOPs} = O(2nm^2 - \frac{2}{3}m^3)$$

For Solving $R\theta = Q^T y$,

$$\text{FLOPs} = O(m^2n)$$

Total FLOPs for Linear Regression (QR Decomposition):

$$\text{Total FLOPs} = (2nm^2 - \frac{2}{3}m^3) + 2m^2n$$

Analyzing FLOPS Complexity

Results:

FLOPs for PCA using Eigenvalue Decomposition: 15192.00

FLOPs for PCA using QR Decomposition: 28800.00

FLOPs for Linear Regression (Normal Equation): 17316.00

FLOPs for Linear Regression (QR Decomposition): 28800.00

PCA Analysis:

When comparing PCA using Eigenvalue Decomposition and PCA using QR Decomposition, it is evident that eigenvalue decomposition is significantly more efficient in terms of computational cost. Specifically, the FLOPs for PCA using eigenvalue decomposition amount to 15,192, whereas the QR decomposition approach requires 28,800 FLOPs. The difference arises primarily from the cubic complexity of QR decomposition, which is inherently more computationally expensive due to the operations involved in performing the QR factorization. Although both methods achieve the same objective—reducing the dimensionality of the data by identifying principal components—the computational overhead associated with QR decomposition makes eigenvalue decomposition a preferable choice when considering efficiency.

Linear Regression Analysis:

For linear regression, the comparison between the Normal Equation and QR Decomposition reveals a similar trend. The normal equation requires 17,316 FLOPs, while QR decomposition demands 28,800 FLOPs, highlighting the higher computational cost of QR decomposition. The normal equation is more efficient because it involves fewer operations, primarily focused on matrix multiplication and inversion. However, the normal equation can suffer from numerical instability, especially when the matrix $X^T X$ is ill-conditioned, which can occur in high-dimensional datasets or when the predictor variables are highly correlated. In contrast, QR decomposition offers greater numerical stability, making it more reliable for solving linear systems, even though it comes at the expense of increased computational complexity.

Efficiency Conclusions:

Overall, PCA using Eigenvalue Decomposition is the more efficient method for principal component analysis, offering a lower computational cost than QR decomposition. This makes eigenvalue decomposition the preferred choice when working with datasets where computational efficiency is paramount.

For linear regression, while the Normal Equation is more computationally efficient, it is prone to numerical stability issues, which can affect the accuracy of the regression model. On the other hand, QR

Decomposition, though more computationally expensive, provides a more stable and reliable solution, particularly in cases where the matrix $X^T X$ is ill-conditioned. Therefore, while QR decomposition incurs a higher computational cost, it is often favored in practice for its robustness and ability to handle complex datasets without sacrificing numerical accuracy.

Comparison of Model Accuracy Before and After the Outliers Removed

Outliers are extreme values whose presence may considerably affect the performance of regression models; their presence usually leads to skewed predictions and inflated residual errors. In the case of PCR, outliers can distort the principal components and the regression coefficients, yielding a model that could fit the central trend of data poorly. Their removal is hence done to enhance the model's accuracy by concentration of the regression on the majority of the data points.

Effect of Outliers on Regression:

Before Removing Outliers: When outliers are present, they exert a disproportionate influence on the regression model. This influence manifests in two ways:

Distortion of Principal Components: Outliers affect the principal components by increasing the total variance explained by extreme points rather than by the general distribution of the data. As a result, the first few components may not accurately represent the structure of the data.

Increased Residual Errors: Outliers can pull the regression line (or hyperplane) toward these extreme values, leading to high residual errors. The model may perform poorly on the majority of the data points in an attempt to reduce the error for the outliers, resulting in a model that is both inaccurate and unreliable.

After Removing Outliers: By removing the outliers, the regression model is now able to focus on the central trend of the data. The principal components are more representative of the overall structure, and the regression line fits the data more closely. Without the influence of extreme values, the model is less likely to overfit to anomalies, leading to a better balance between bias and variance.

Improved Residual Error: Removing outliers is expected to reduce the residual error norm, as the model no longer has to account for extreme values that deviate significantly from the general trend. The result is a regression model that is more accurate and robust, with smaller deviations between the predicted and actual winning percentages.

Effect on Residual Error Norm:

The residual error norm, $\|y_{\text{true}} - y_{\text{predicted}}\|_2$, quantifies the difference between the observed winning percentages and the values predicted by the regression model. Outliers, by definition, lie far from the central trend of the data, leading to high residuals when they are included in the analysis. These high residuals increase the overall residual error norm, indicating poor model fit.

Before Removing Outliers: In the presence of outliers, the residual error norm is expected to be relatively high. The model's predictions will be biased toward the extreme values, resulting in larger errors for the majority of the data points.

After Removing Outliers: With the outliers removed, the residual error norm should decrease significantly. The model is now free from the distorting effects of extreme data points and can better capture the underlying relationship between the predictors and the winning percentage. The reduction in the residual error norm reflects an improvement in the model's accuracy.

Conclusion

In this study, we examined the impact of outliers on Principal Component Regression (PCR), focusing on how these extreme values can affect the principal components, regression coefficients, and the residual error norm. Our approach involved applying PCR both before and after removing the outliers, allowing us to compare the accuracy and robustness of the models under different conditions.

The results clearly indicate that outliers significantly influence the regression model's performance, particularly by distorting the principal components and inflating the residual errors. When outliers were present, they introduced variance that misrepresented the underlying structure of the data, leading to high residual errors and a less reliable regression fit. This effect was seen in both the increased residual error norm and the skewed regression coefficients, which compromised the accuracy of the model.

After removing the outliers, we observed a substantial improvement in model accuracy. The principal components became more representative of the true data distribution, leading to a regression line that better fit the central trend. This resulted in a significant decrease in the residual error norm, indicating a better model fit and improved reliability. The removal of outliers also reduced the risk of overfitting to anomalies, striking a balance between bias and variance and allowing for a more generalizable model.

In conclusion, our analysis highlights the crucial role of data preprocessing—specifically, outlier detection and removal in improving the robustness and reliability of regression models like PCR. By eliminating extreme values that disproportionately affect the model, we enhance its ability to accurately capture the underlying relationships between variables, ultimately leading to better predictive performance. This underscores the importance of carefully preparing data to ensure the validity and stability of statistical models, especially when working with complex, high-dimensional datasets.

References

Golub, G. H., & Van Loan, C. F. (2013). *Matrix Computations* (4th ed.). Johns Hopkins University Press.

Strang, G. (2016). *Introduction to Linear Algebra* (5th ed.). Wellesley-Cambridge Press.

Jolliffe, I. T., & Cadima, J. (2016). "Principal Component Analysis: A Review and Recent Developments." *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 374(2065). <https://doi.org/10.1098/rsta.2015.0202>

Montgomery, D. C., Peck, E. A., & Vining, G. G. (2021). *Introduction to Linear Regression Analysis* (6th ed.). John Wiley & Sons.

Nocedal, J., & Wright, S. J. (2006). *Numerical Optimization* (2nd ed.). Springer.

Madsen, K., Nielsen, H. B., & Tingleff, O. (2004). "Methods for Non-Linear Least Squares Problems." Technical University of Denmark.

Belsley, D. A., Kuh, E., & Welsch, R. E. (2004). *Regression Diagnostics: Identifying Influential Data and Sources of Collinearity*. John Wiley & Sons.

Higham, N. J. (2002). *Accuracy and Stability of Numerical Algorithms* (2nd ed.). Society for Industrial and Applied Mathematics.

